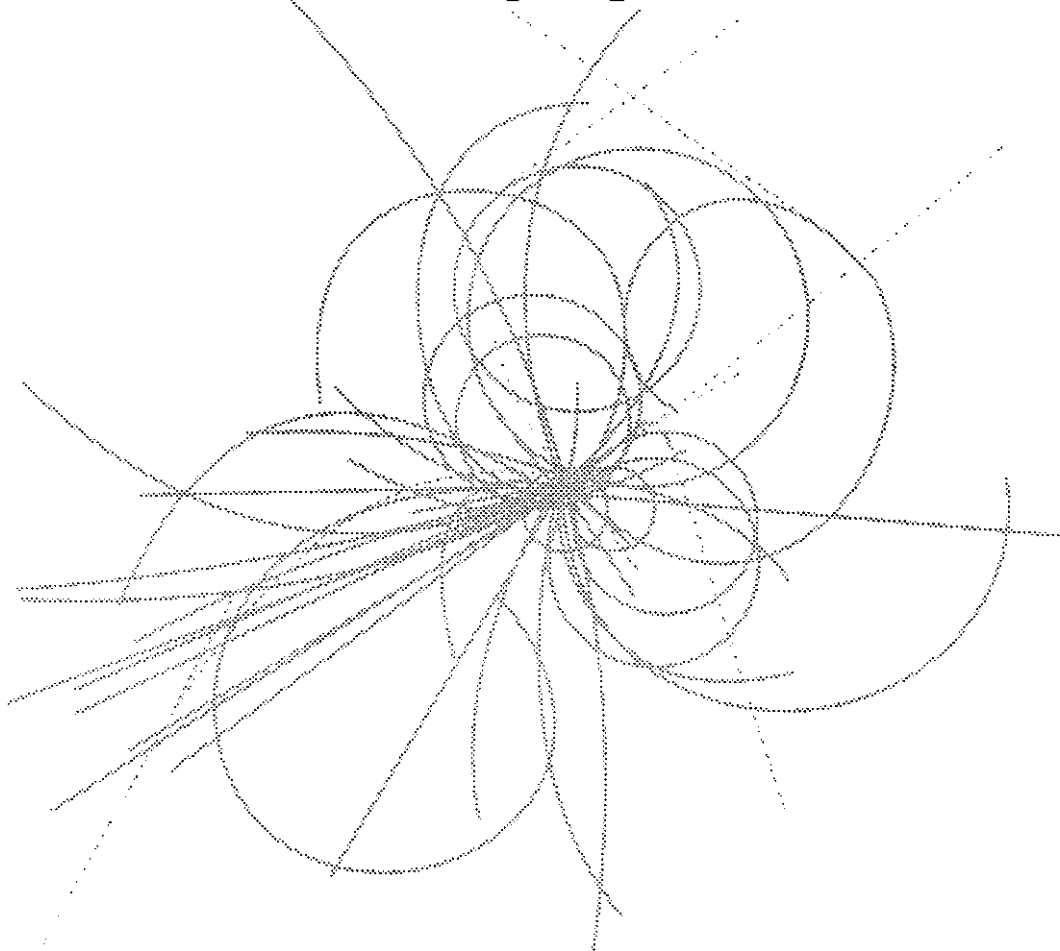


Superconducting Super Collider Laboratory



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J. Rasson and J. Dweck

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August 1990

*Presented at the International Industrial Symposium on the Super Collider, Miami Beach, Florida, March 14-16, 1990.

[†]Operated by the Universities Research Association, Inc., for the U.S. Department of Energy under Contract No. DE-AC02-89ER40486.

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INTRODUCTION

The SSC Magnet must maintain at a super conducting temperature of 4 K. The proposed refrigeration cooling processes consist of fairly simple closed cycles which take advantage of the Joule-Thompson effect via a series of expansions and compressions of helium gas which has been precooled by liquid nitrogen. The processes currently under consideration consist of three cycles, the 20 K shield cooling, the 45 K helium refrigerator and the helium liquefier. The process units which are to be employed are compressors, turbines, expanders, mixers, flashes, two stream heat exchangers and multiple stream heat exchangers. The cycles are to be operated at or near steady state.

Due to the large number of competing cooling sector designs to be considered and the high capital and operating costs of the proposed processes, the SSC Laboratory requires a software tool for the validation and optimization of the individual designs and for the performance of cost-benefit analyses among competing designs. Since these processes are steady state flow processes involving primarily standard unit operations, a decision was made to investigate the application of a commercial process simulator to the task.

Several months of internal evaluations by the SSC Laboratory revealed that while the overall structure and calculation approach of a number of the commercial simulators were appropriate for this task, all were lacking essential capabilities in the areas of thermodynamic property calculations for cryogenic systems and modeling of complex, multiple stream heat exchangers. An acceptable thermodynamic model was provided and a series of simple, but

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representative benchmark problems developed. The model and problems were provided to three software vendors. Based on the results of the benchmark tests, the ASPEN/SP process simulator was selected for future modeling work.

ENHANCEMENT OF THE ASPEN/SP PROCESS SIMULATOR

While ASPEN/SP process simulator has the basic flowsheeting capabilities and unit operation models required for this task, several enhancements were needed to facilitate development of the SSC process models. These enhancements can be classified into three categories: thermodynamic models, two-phase flash algorithm, and unit operation models. Each is discussed below.

Thermodynamic Models

Unlike most chemical processes, the SSC cooling sector involves the flow of only pure components. Essentially pure helium is the fluid used in the cycles, while pure nitrogen is used external to the cycle to cool the helium to the maximum temperature at which JouleThompson cooling can take place. While the lack of mixtures should simplify the physical property calculations, the peculiarities of helium actually lead to greater physical property problems than for even fairly complex chemical systems.

Nitrogen does not exhibit any unusual behavior and, as such, is fairly easily modeled via conventional equations of state. For the purposes of this work, a highly accurate 32-term variation of the BWR equation of state developed by¹ Jacobsen is employed. This equation is valid from 63.15 to 1900 K and pressures up to 1000 bar. The uncertainties in the calculated temperatures are under 0.5% while the enthalpy is within 3.0 joules/k-mole across the entire range. Calculation times are fairly long owing to the difficult nature of the root finding procedure for this equation.

Helium exhibits phase, enthalpy and transport behavior unlike any other substance. Liquid helium forms two distinct phases, the normal fluid and the superfluid. The specific heat decreases with temperature to about 2.5 K, then increases dramatically to the lambda point (2.172 K), then decreases dramatically. The thermal conductivity of the normal fluid actually decreases with decreasing temperature, which is similar to the behavior of a gas. On the other hand, the thermal conductivity of the superfluid is so high, that bubble formation cannot take place during boiling. The superfluid also displays a behavior termed superfluidity, where it acts as if it had zero viscosity.

To provide for the simulation of the proposed cycles, a physical property model capable of accurately calculating the liquid and vapor phase fugacities, enthalpies, entropies and densities of helium at temperatures from 0.8 K to 500 K and pressures up to 3,000,000 N/sqm is required. Since the majority of the proposed designs operate above the lambda temperature of helium (2.172 K), the first model which was implemented is the well-known² McCarty model, distributed by the National Bureau of Standards. This model was designed as a standalone program for the calculation of vapor and liquid helium properties. While the model can accept various input specifications, the only specifications which are useful for ASPEN/SP are temperature and pressure.

When the temperature and pressure are specified, the model determines the phase of the helium and returns a list of properties, including density, enthalpy, entropy and heat capacity. In ASPEN/SP, however, the flash algorithm is responsible for determining the phase of the system. In order to make this determination, the flash algorithm requires the fugacity and enthalpy of both the liquid and vapor phases at the specified condition. If the system does not exist in one of the states at the condition, extrapolated hypothetical values must be returned by the physical property models. Since the McCarty model is not designed to return data for hypothetical phases, modifications had to be made.

The equation of state has multiple roots, two of which represent either the actual or extrapolated liquid and vapor roots. The root finding algorithm of the original McCarty model, which employs a Newton-Raphson approach, is not robust enough to locate the extrapolated root in the general case. The cause of this problem was isolated to the division of the temperature-pressure plane into four regions, each with different coefficients, to enhance the accuracy of the model. The function is not smooth across the boundaries, limiting the effectiveness of the Newton-Raphson algorithm when the boundaries are crossed. This problem was solved by modifying the Newton-Raphson algorithm to use the analytical derivatives to calculate an approximate next value of the iteration variable, then recalculating the derivative numerically via finite difference between the new point and the original point. This derivative then is used by the Newton-Raphson technique to determine the actual new value. This approach while only slightly slower does eliminate the robustness problems.

For temperatures below the lambda point, a proprietary model developed by Air Products was implemented. This model also appears to perform reliably above the lambda point, although errant phase determinations did result when applying this model near the critical point. This problem was not observed with the ASPEN/SP implementation of the McCarty model. The two models are implemented in such a fashion that the user can select either model by setting a single input parameter.

Two-Phase Flash Algorithm

The two phase flash algorithm contained in ASPEN/SP is extremely robust and efficient for a wide variety of chemical systems over broad ranges of temperature and pressure. However, in order to accommodate the temperature range encountered in the proposed cooling sector designs and the temperamental nature of the McCarty thermodynamic model, two minor modifications were required. First, the lower temperature bound was changed from 50 K to 2.1 K. (For the later work, the bound was lowered to 0.5 K.) Second, functions were developed to aid in the generation of initial temperature estimates for specified pressure - enthalpy flashes.

The initial estimate functions are necessary because of the highly irregular nature of the enthalpy of the hypothetical vapor root solution to the McCarty equation. In certain circumstances, the enthalpy of the hypothetical vapor actually will decrease with increasing temperature. This can cause the erroneous calculation of a high temperature vapor instead of a low temperature liquid at a particular pressure and enthalpy if a poor initial temperature estimate is selected. The initial estimate functions are based on regressed fits of the saturated liquid and vapor enthalpies of helium as a function of pressure.

Unit Operation Models

In addition to the two-phase flash algorithm enhancement described above, three unit operation enhancements were required to simulate the proposed designs. These three enhancements involve the development of user subroutines to facilitate off-design calculations with the turbine, robustness improvements for the two stream heat exchanger and the development of a multiple stream heat exchanger model. Each of these enhancements is discussed below.

When a turbine is operated at other than the design pressures and flow rate, the efficiency is different from the design efficiency. This variation in efficiency is described via a turbine curve. The user subroutines function by calculating the inlet nozzle diameter for the turbine at the design condition, assuming choke flow. The efficiency in off-design conditions then is computed as a fraction of the design efficiency via a look-up of a turbine curve at the desired condition, given the inlet nozzle diameter. A subroutine which calculates the speed of sound in helium was developed to facilitate this calculation.

The two-stream heat exchanger algorithm needed minor enhancements to handle certain types of phase transitions in the helium and to facilitate heat leak calculations. For chemical systems involving mixtures, the system must pass through a two-phase region between the vapor and liquid states. For pure components, however, a supercritical fluid which is at a pressure above the critical pressure, and is cooled at constant pressure can undergo an immediate transition to a saturated liquid without passing through the two-phase region. This behavior is observed in several of the heat exchangers and necessitated a modification to the two stream heat exchanger phase transition logic. The exceedingly low temperatures and odd geometries of the heat exchanger necessitate a provision for heat leak calculations. A capability to specify either a positive or negative heat leak as a fraction of the total heat transferred was added to the two-stream heat exchanger model.

A significant amount of effort was expended in the design of a multiple stream heat exchanger algorithm. Multiple stream heat exchangers are quite complex, involving the splitting of each feed stream into a number of flows which are exchanged in a countercurrent fashion against the opposite feed streams in a series of channels. Each hot stream flow contacts two cold stream flows simultaneously and visa versa. A certain fraction of the heat exchanger areas is devoted to each type of exchange.

Two algorithms were designed to model these exchangers. The first considers the area distribution inside the exchanger and simultaneously calculates the various types of exchanges, combining the outlet flows to achieve the final temperatures. The second is a highly simplified algorithm, referred to as the lumped-approach, which considers the exchanger to be a series of two stream heat exchangers. At the cold side, the coldest feed stream is heated against the combined hot streams, until the stream reaches the temperature of the next coldest feed stream. At this point, the two cold streams together are heat exchanged against the combined hot streams. The hot streams are treated analogously. That is, the hottest stream is cooled against the combined cold streams until the stream reaches the temperature of the next hottest stream. At this point, the two hot streams together are exchanged against the combined cold streams.

For the purposes of this work, the simplified, lumped-approach algorithm was adopted. This approach imposes a number of limitations upon the model, including the

uniformity of outlet temperatures on each side, the specification of a single heat transfer coefficient for all phase regimes, imprecise determination of pinch-point conditions, and limited applicability to off-design and rating situations. Independent specification of pressures and physical property methodology for individual streams are allowed and have been implemented.

The algorithm which has been implemented has a great deal of flexibility, allowing the specification of either the hot or cold stream outlet temperature, the exchanger duty, the minimum approach temperature or the overall exchanger area. The algorithm begins by calculating the overall heat duty and temperature at which each of the streams on either side begin to participate in the heat exchange. The first three types of specifications then are straightforward, involving no iterative calculations. The overall heat duty is the primary iteration variable for the minimum approach and area specifications. The heat duty is a superior iteration variable to the temperature due to the linear nature of the convergence and the elimination of convergence difficulties associated with phase transitions of pure components.

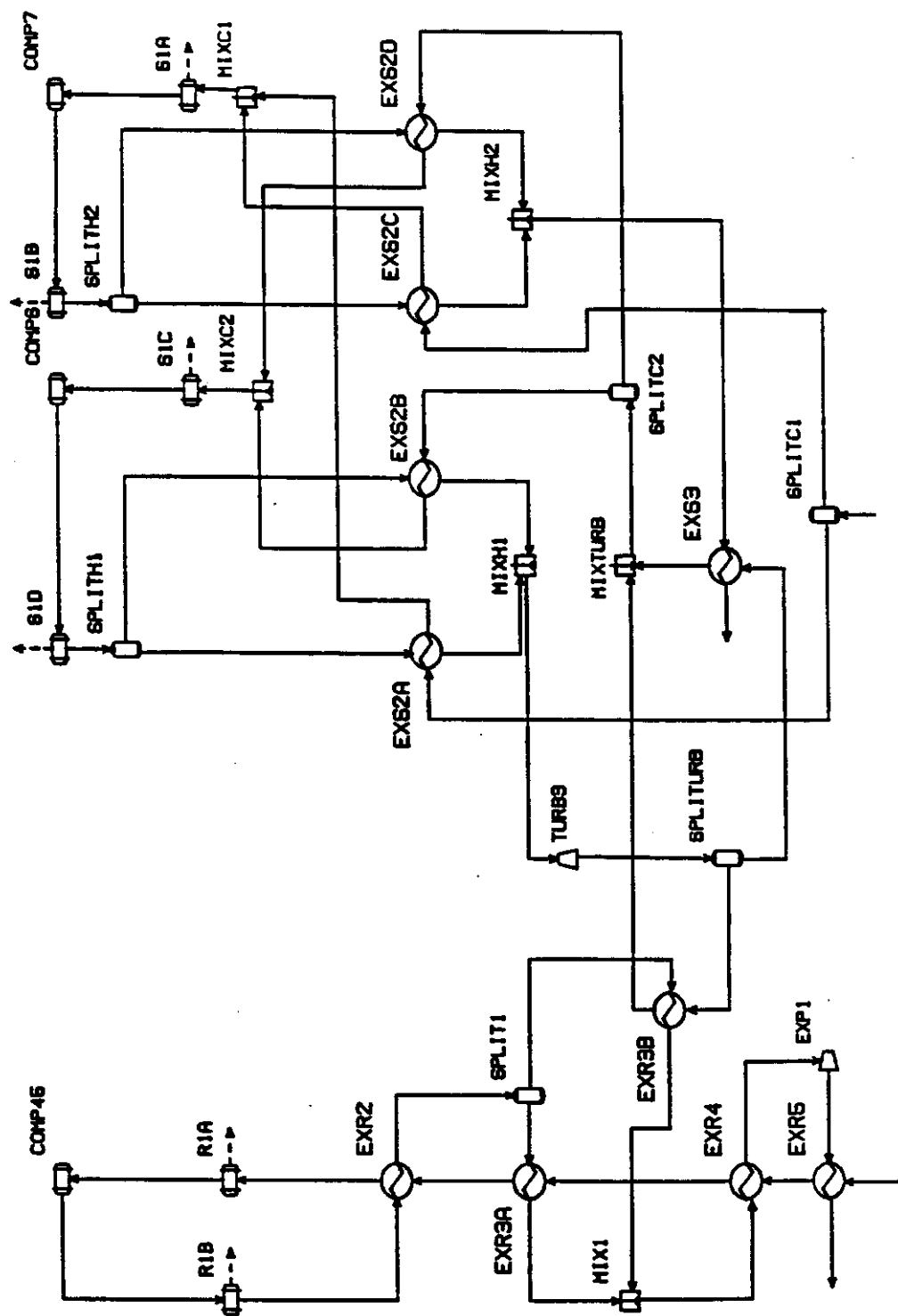
The multiple stream heat exchanger algorithm has performed very well, converging reliably and efficiently for all of the cases which have been tried. All of the specification options have been exercised and shown to produce consistent results.

EXAMPLE APPLICATION

While most of the cooling sector designs which have been simulated are proprietary, the simulation of a sample design can be discussed. Figure 1 is a simulation flowsheet of the combined 20 K shield and 4 K refrigerator for the sample design. This flowsheet contains ten two stream heat exchangers and assorted compressors, turbines and heaters. The nitrogen precooling has been neglected and the multiple stream heat exchangers have been represented as groups of two stream heat exchangers.

The ASPEN/SP input file for this simulation is contained in Figure 2. The special cryogen physical property option set has been employed. The simulation is performed in rating mode, with the areas of each of the heat exchangers being specified. Since the flowsheet forms a series of complex loops, tear streams have been specified and estimated flow rates and phase conditions specified. The tear streams are to be converged simultaneously.

Representative simulation results are contained in Figures 3 and 4. Figure 3 is a plot of the temperature profile in heat exchanger EXR5, which subcools a high pressure liquid stream against a low pressure vapor stream. The pronounced curvature of the hot stream cooling curve results from the unusual temperature variation of the helium heat capacity in the near-critical region. Figure 4 is a plot of the temperature difference profile in exchanger EXR5. The peak in this curve results from the curvature of the hot stream cooling curve. Figure 5 is an excerpt of the stream report for the simulation which contains the hot outlet stream from exchanger EXRS. The tear streams were converged in nine overall flowsheet iterations in approximately four hours on a 16 MhZ, 386 PC.



ASPEN/SP-PC - JSD Simulation Services

Figure 1. Simulation flowsheet of combined 20K shield and 4K refrigerator.


```

BLOCK SPLITC2 IN = 234          OUT = 234A 234B
BLOCK MIXC2 IN = 232A 232B      OUT = 232
BLOCK SPLITC1 IN = 224          OUT = 224A 224B
BLOCK SPLITH1 IN = 242          OUT = 242A 242B
BLOCK MIXH1 IN = 244A 244B      OUT = 244
BLOCK SPLITH2 IN = 212          OUT = 212A 212B
BLOCK MIXH2 IN = 214A 214B      OUT = 214
BLOCK EXS3 IN = 214 256         OUT = 216 254
BLOCK S1A IN = 222              OUT = 220 QS1A
BLOCK S1B IN = 210              OUT = 212 QS1B
BLOCK S1C IN = 232              OUT = 230 QS1C
BLOCK S1D IN = 240              OUT = 242 QS1D
BLOCK COMP7 IN = 220            OUT = 210
BLOCK COMP6 IN = 230            OUT = 240
BLOCK MIXTURE IN = 254 235      OUT = 234
BLOCK TURB3 IN = 244            OUT = 246

;
;BLOCKS PARAGRAPH 4K REFER
;
BLOCK SPLITURB FSPLIT
  FRAC 256 .6521
  BOPT HNB-RESULTS=0
;
BLOCK EXR5 HEATX
;SUBROUTINE UHEQ2M
  PARAM 5 0 AREA=4.1343 DPC=-0.01 DPH=-0.05
;
  FLASH-SPECS 172 NPK=1 KPH=2
  FLASH-SPECS 128 NPK=1 KPH=1
  REPORT CURVES
;
BLOCK EXP1 COMPR
  PARAM TYPE=3 PRES=2.05 ES=.7377
;
BLOCK EXR4 HEATX
;SUBROUTINE UHEQ2M
  PARAM 5 0 AREA=20.1219 DPC=-.01 DPH=-.1
  BOPT RESTART=0
  FLASH-SPECS 118 NPK=1 KPH=1
  FLASH-SPECS 126 NPK=1 KPH=1
  REPORT CURVES
;
BLOCK MIX1 MIXER
;
BLOCK EXR3A HEATX
;SUBROUTINE UHEQ2M
  PARAM 5 0 AREA=10.7292 DPC=-.02 DPH=-.1
  FLASH-SPECS 116A NPK=1 KPH=1
  FLASH-SPECS 124 NPK=1 KPH=1
  REPORT CURVES
;
BLOCK EXR3B HEATX
;SUBROUTINE UHEQ2M
  PARAM 5 0 AREA=5.5104 DPC=-.02 DPH=-.1
  FLASH-SPECS 116B NPK=1 KPH=1
  FLASH-SPECS 235 NPK=1 KPH=1
  REPORT CURVES
;
BLOCK SPLIT1 FSPLIT
  FRAC 114B .34973
  BOPT HNB-RESULTS=0

```

Figure 2. ASPEN/SP simulation input file (continued).

```

;
BLOCK EXR2 HEATX
;SUBROUTINE UHE02N
PARAM 5 0 AREA=59.6061 DPC=-.02 DPH=-.1
FLASH-SPECS 114 NPK=1 KPN=1
FLASH-SPECS 122 NPK=1 KPN=1
REPORT CURVES
;
BLOCK R1A HEATER
PARAM PRES=-.04 TEMP=300.
;
BLOCK R1B HEATER
PARAM PRES=-.1 TEMP=80.
;
BLOCK COMP45 HEATER
PARAM PRES=18 TEMP=300.
;
;
;BLOCKS PARAGRAPH 20K REFER
;
BLOCK EXS2A HEATX
;SUBROUTINE UHE02N
PARAM 5 0 AREA=6.2137 DPC=-.05 DPH=-.1
FLASH-SPECS 222A NPK=1 KPN=1
FLASH-SPECS 244A NPK=1 KPN=1
REPORT CURVES
;
BLOCK EXS2B HEATX
;SUBROUTINE UHE02N
PARAM 5 0 AREA=119.0726 DPC=-.03 DPH=-.1
FLASH-SPECS 232B NPK=1 KPN=1
FLASH-SPECS 244B NPK=1 KPN=1
REPORT CURVES
;
BLOCK EXS2C HEATX
;SUBROUTINE UHE02N
PARAM 5 0 AREA=50.473 DPC=-.05 DPH=-.05
FLASH-SPECS 222B NPK=1 KPN=1
FLASH-SPECS 214A NPK=1 KPN=1
REPORT CURVES
;
BLOCK EXS2D HEATX
;SUBROUTINE UHE02N
PARAM 5 0 AREA=5.6267 DPC=-.03 DPH=-.05
FLASH-SPECS 232A NPK=1 KPN=1
FLASH-SPECS 214B NPK=1 KPN=1
REPORT CURVES
;
BLOCK SPLITC1 FSPLIT
FRAC 224B .90
BOPT HMB-RESULTS=0
;
BLOCK SPLITC2 FSPLIT
FRAC 234B .9495
BOPT HMB-RESULTS=0
;
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FRAC 242B .9440
BOPT HMB-RESULTS=0
;

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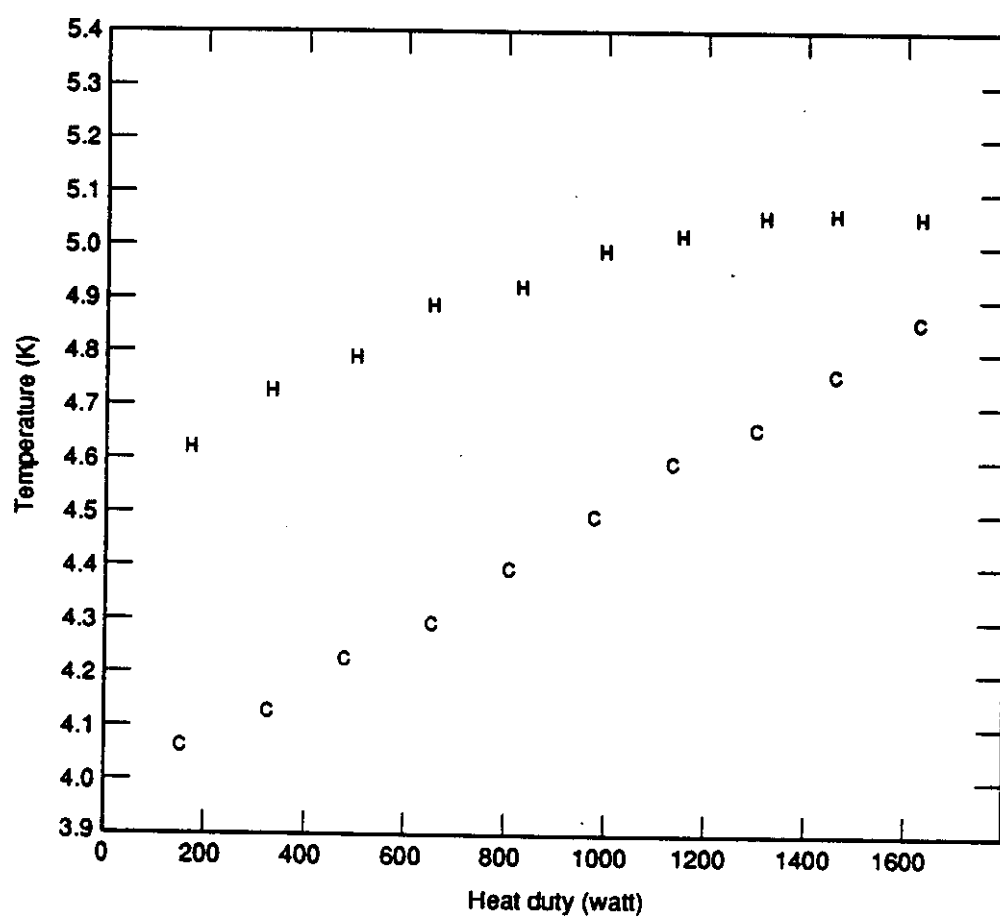
Figure 2. ASPEN/SP simulation input file (continued).

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  FRAC 212A .9094
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;
;
BLOCK MIXN1 MIXER
;
BLOCK MIXC1 MIXER
;
BLOCK MIXN2 MIXER
;
BLOCK MIXC2 MIXER
;
BLOCK EXS3 HEATX
  ;SUBROUTINE UME02N
  PARAM 5 0 AREA=15.3040 DPC=-.02 DPN=-.05
  FLASH-SPECS 254      NPK=1  KPH=1
  FLASH-SPECS 216      NPK=1  KPH=1
;
BLOCK S1A HEATER
  PARAM PRES=-.05 TEMP=300.
;
BLOCK S1B HEATER
  PARAM PRES=-.1 TEMP=80.
;
BLOCK S1C HEATER
  PARAM PRES=-.05 TEMP=300.
;
BLOCK S1D HEATER
  PARAM PRES=-.1 TEMP=80.
;
BLOCK COMP6 HEATER
  PARAM PRES=8.2 TEMP=300.
;
BLOCK MIXTURB MIXER
;
BLOCK COMP7 HEATER
  PARAM PRES=2.7 TEMP=300.
;
BLOCK TURB3 COMPR
  PARAM TYPE=3 ES=.76 PRES=2.1
;
;STREAM PARAGRAPH
;
;
;STREAM 236 PRES=2.1 TEMP=16.75 MASS-FLOW=.1319
; MOLE-FRAC HELIUM 1.0
;
;STREAM 182 PRES=.8 TEMP=3.996 MASS-FLOW=.24892
; MOLE-FRAC HELIUM 1.0
;
;STREAM 112 PRES=17.9 TEMP=80 MASS-FLOW=.24892
; MOLE-FRAC HELIUM 1.0
;
;STREAM 114 PRES=17.8 TEMP=25.5 MASS-FLOW=.24892
; MOLE-FRAC HELIUM 1.0
;
;STREAM 116 PRES=17.7 TEMP=17.5 MASS-FLOW=.24892

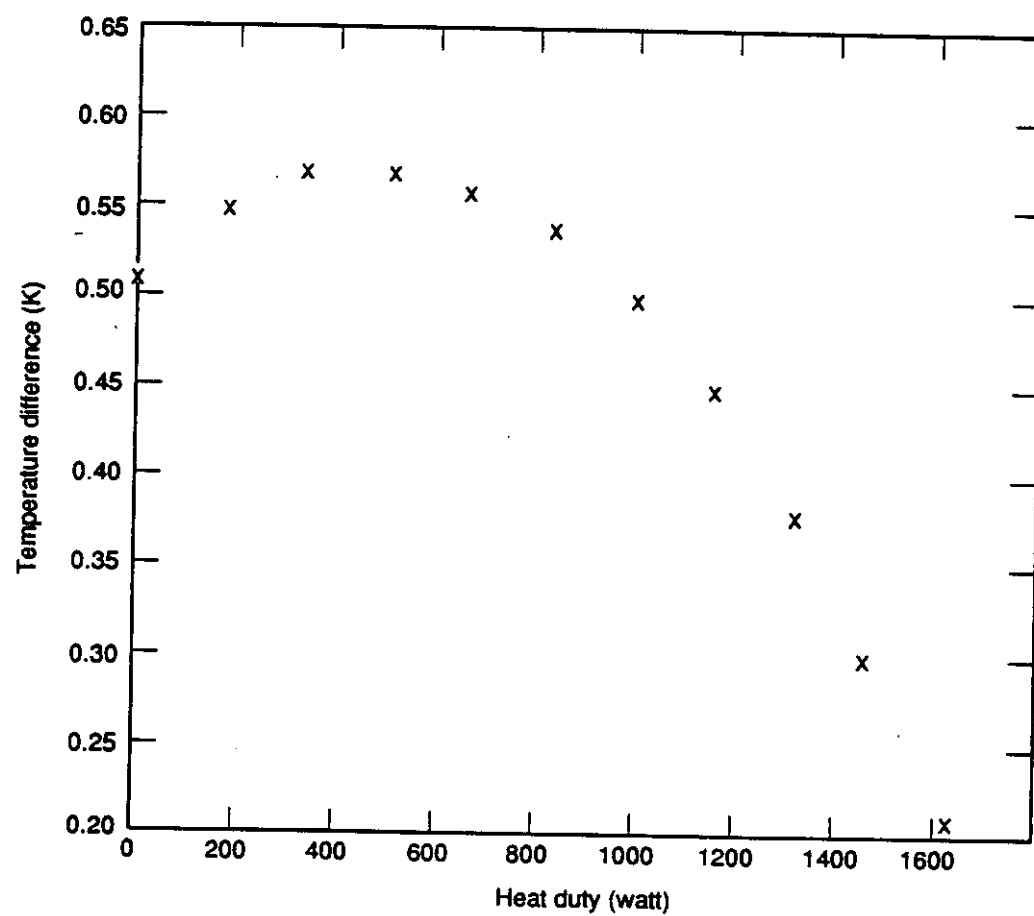
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Figure 2. ASPEN/SP simulation input file (continued).



TIP-01175

Figure 3. Plot of Temperature Profile in Heat Exchanger EXR5.



TIP-01176

Figure 4. Plot of Temperature Difference Profile in Heat Exchanger EXR5.

ASPEN/SP Run On 9/ 4/87 by JSD Simulation Page 178
 ASPEN/SP Version 1.5 Released By JSD, Inc., Denver, Colorado on JUNE 30, 1985
 SIMPLIFIED CRYOGENIC REFRIGERATION CYCLE
 STREAM SECTION

	256	236	172	128
FLOW DETAILS				

COMPONENT FLOWS <KMOL/SEC>				

NITROGEN	0.0	0.0	0.0	0.0
HELIUM	0.0617	0.0329	0.0621	0.0621

TOTAL	0.0617	0.0329	0.0621	0.0621
PHASE SPLITS				

VAPOR FRACTION <MOLE BASIS>	1.0000	1.0000	0.0	1.0000
LIQUID FRACTION <MOLE BASIS>	MISSING	MISSING	1.0000	0.0
SOLID FRACTION <MOLE BASIS>	MISSING	MISSING	0.0	0.0
INTENSIVE PROPERTIES				

TEMPERATURE <K>	16.7322	16.7322	4.5034	4.8731
PRESSURE <ATM>	2.1000	2.1000	2.0000	0.7900
MOLECULAR WEIGHT	4.0030	4.0030	4.0030	4.0030
ENTHALPY <J/KMOL>	-.58562+07	-.58562+07	-.62110+07	-.61100+07
ENTROPY <J/KMOL-K>	-.66360+05	-.66360+05	-.11112+06	-.85263+05
DENSITY <KMOL/CM3>	1.5445	1.5445	31.1068	2.3222

Figure 5. Excerpt of the stream report for the simulation that contains hot water outlet stream from EXR5.

CONCLUSIONS

Our work has demonstrated that reliable, predictive simulation models of the cooling sector of the SSC can be developed with ASPEN/SP. Verification and preliminary optimization of individual designs also has proven feasible via the simulation models. Finally, the simulation models have proven useful for the performance of rudimentary cost-benefit analyses of competing process designs. The ability to perform meaningful off-design and optimization studies is somewhat limited due primarily to the inadequacies of the multiple stream heat exchanger and compressor-turbine unit operation models.

RECOMMENDATIONS FOR FUTURE WORK

While the modeling work has been successful and has served most of the desired purposes, a few additional enhancements would prove quite useful for process optimization and studying the performance at off-design conditions. The first of these enhancements is a simplified equation of state for helium, which executes faster than the McCarty model with no significant loss of accuracy. Air Products has developed a proprietary implementation of such a model, although a thorough study of the accuracy and robustness of the model has not yet been performed. A second desirable enhancement is a compressor - turbine model which is capable of performing fairly sophisticated rating calculations, including the prediction of choke flow conditions and off-design efficiencies. Such a model is essential for off-design simulations. A third recommended enhancement is the addition of an axial heat conduction calculation to the two stream heat exchanger. Axial conduction is significant due to the geometry of the cryogenic exchangers employed. A final recommended enhancement is a more rigorous multiple stream heat exchanger model, which considers the area distribution inside the exchanger. Such a model would be very useful in optimizing heat exchanger design and in predicting off-design performance.

REFERENCES

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2. McCarty, R. D., Thermodynamic Properties of Helium 4 from 2 to 1500 K at Pressures to 10^8 Pa, J. Phys. Chem. Ref. Data 2, No. 4, 923-1042 (1973)